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VARIATIONAL TREATMENT OF SLOW ELECTRON SCATTERING BY A HELIUM ATOM

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ABSTRACT The scattering of slow electrons by a helium atom has been investigated with allowance for exchange possibility and polarisation effects. Using a two-parameter open shell wave function for the ground state of helium, the S-wave shifts for several incident electron energies have been calculated by the well-known variational method of Hulthén (1944). The close agreement of our zero-energy cross section with the exact calculations of Williamson and McDowell (1965) shows the correctness of validity of the variational method for this problem. It may be added that our result also agrees well with the experimental values of Bandel and Golden (1965).

INTRODUCTION

Recently experimental results of Pack, Phelps *et al* (1961, 1964) and of Bandel and Golden (1965) indicate agreement with theoretical findings much closer than what was possible before; in view of this we have tried in this paper to find out whether the same agreement is obtainable with variational method.

The first theoretical investigation of the elastic scattering of electrons by helium atom has been carried out by Massey and Mohr (1931) with the inclusion of exchange possibilities and exclusion of polarisation effects. They found that the exchange effect was quite important below 15 ev incident electron energy. Under the same assumption regarding polarisation and exchange, Allis and Morse (1933) have determined S and P wave phase shifts by exact numerical solution of integro-differential equation. Moisseiwitsch (1953) using a closed-shell wave function of helium atom, has calculated the same elastic cross-section using Hulthen's variational method and under the same assumption. Adopting an open-shell wave function of the helium atom, similar calculations have been done numerically by Moiseiwitsch (1961). On the other hand, taking an open-shell wave function, Mukherjee and Sil (1962) have obtained almost the same value of zero-energy cross-section as that of Moiseiwitsch (1961).

LaBahn and Callaway (1964) in their numerical calculation with Hartree-Fock separable ground state wave function have found that the influence of polarisation effect considerably lowers the theoretical zero-energy cross-section towards much better agreement with the experimental value; however, the theoretical

value is somewhat a little less than the experimental one Williamson and McDowell (1965) have recalculated the same problem numerically with an open-shell wave-function for helium atom Their findings for the zero-energy cross-section is almost the same as that of LaBahn and Callaway (1964)

In this paper we have applied Hulthen's variational method to calculate the S-wave phase-shifts for electron-helium atom elastic scattering taking into account both exchange and polarisation effects, we have used the same open-shell wave function as used by Williamson and McDowell (1965). The value of our zero energy cross section is 16 33 a^2 as against 16.10a^2 and 16 50a^2 of LaBahn and Callaway (1964) and Williamson and McDowell (1965) respectively

THEORY

The system of helium atom and the incident electron satisfies the wave equation,

$$(H-E)\ \psi(r_1, r_2, r_3) = 0 \qquad \ldots \quad (1)$$

where H and E are the total Hamiltonian and energy of the system respectively The Hamiltonian is given by

$$H = -\nabla_1^2 - \nabla_2^2 - \nabla_3^2 - \frac{4}{r_1} - \frac{4}{r_2} - \frac{4}{r_3} + \frac{2}{r_{12}} + \frac{2}{r_{13}} + \frac{2}{r_{23}}, \quad E = K_0^2 + E_0$$

and r_1, r_2, r_3 are the distances of the three electrons from the nucleus of the helium -atom, r_{12}, r_{23}, r_{13} are the distances between the electrons, E_0 being the ground - state energy of the atom (in Rydberg units) and K_0 is the wave number of the incident electron (unit of length being the Bohr radius a_0).

Let $\psi(r_1, r_2, r_3)$ be approximated by the following expansion

$$\psi(r_1, r_2, r_3) = F_0(r_1)\psi_0(r_2, r_3)\,\chi(1, 2, 3) + F_0(r_2)\psi_0(r_3, r_1)\,\chi(2, 3, 1) + F_0(r_3)\psi_0(r_1, r_2)\,\chi(3, 1, 2) \qquad \ldots \quad (2)$$

where $F_0(r)$ is a function describing the free electron,

$\psi_0(r_1, r_2)$ is the singlet ground state wave function of the He-atom and is taken equal to $N(e^{-\lambda r_1 - \mu r_2} + e^{-\mu r_1 - \lambda r_2})$ with $\lambda = 2\ 1832$, $\mu = 1\ 1886$ and $N = 708991$ $\chi(1\ 2,3)$ is a doublet three-electron spin function and is equal to $\frac{1}{\sqrt{2}}\,\alpha_1(\alpha_2\beta_3 - \alpha_3\beta_2)$, α and β being the spin function for an individual electron The above expansion of ψ is anti-symmetric with respect to the interchange of any pair of electrons and hence it takes into account the exchange effect.

Substituting (2) in (1) and multiplying by $1/\sqrt{2}(\alpha_1\beta_2 - \alpha_2\beta_1)\alpha_3$ and summing over the spin co-ordinates and integrating with respect to r_1 and r_2, we obtain

$$[\nabla_3^2 + K_0^2 - V_{00}(r_3)]F_0(r_3) = \iint F_0(r_1)\,P_{00}(r_1, r_2, r_3)dr_1dr_2 \qquad \ldots \quad (3)$$

where $V_{00}(r_3)$ the static potential and is equal to

$$-g\left(\frac{1}{r_3}+\lambda\right)e^{-2\lambda r_3}-g\left(\frac{1}{r_3}+\mu\right)e^{-2\mu r_3}-2h\left(\frac{1}{r_3}+\frac{\lambda+\mu}{2}\right)e^{-(\lambda+\mu)r_3}$$

where $g = 1.13573$ and $h = .864273$

$$P_{00}(r_1, r_2, r_3) = \psi_0(r_2, r_1)\nabla_1^2\psi_0(r_1, r_2)+\psi_0(r_1, r_2)\nabla_2^2\psi_0(r_2, r_3)+\psi_0(r_1, r_2)\nabla_3^2\psi_0(r_2, r_3)$$

$$+\psi_0(r_1, r_2)\psi_0(r_2, r_3)\left[\frac{4}{r_1}+\frac{4}{r_2}+\frac{4}{r_3}-\frac{2}{r_{12}}-\frac{2}{r_{23}}-\frac{2}{r_{13}}+E\right]$$

We expand the wave function of the free-electron in zonal harmonics as

$$F_0(r_3) = \frac{1}{r_3}\sum_{l=0} f_l(r_3)\,\rho_l(\cos\theta_3) \qquad \ldots (4)$$

where $f_l(0) = 0$ and $f_l(r) \sim \sin\left(Kr-\frac{l\pi}{2}+\eta_l\right)$ $r\to\infty$

η_l being the phase-shift.

Substituting $F_0(r)$ from (4) into (3) and multiplying both sides by $P_l(\cos\theta_3)\sin\theta_3\,d\theta_3$ and integrating over the space we get finally

$$\frac{d^2}{dr_3^2}+k_0^2-V_{00}(r_3)-\frac{l(l+1)}{r_3^2}\Big]\,f_l(r_3)$$

$$=\int_0\int_0 Q_{00}(r_1, r_2, r_3)\,f_l(r_1)\,dr_1\,dr_2 \qquad \ldots (5)$$

where

$$Q_{00}(r_1, r_2, r_3) = 16\pi^2 r_1 r_2^2 r_3 P_{00}(r_1, r_2, r_3).$$

LaBahn and Callaway (1964) considering the distortion of the atomic wave function induced by the incoming electron, have obtained in addition to the usual static coulomb potential, a term of the type $\frac{-\alpha(r)}{r^4}$ in the asymptotic region which represents the polarisation effect. For the general case they assume α to be a function of r of the form as obtained by Bethe (1943). With that picture in mind, Williamson and McDowell (1965) have taken the total potential as $V_{00}(r)-\frac{\alpha(r)}{r^4}$ where $\alpha(r)$ is the same as above, though $V_{00}(r)$ is different from that of LaBahn and Callaway (1964). In our calculation, we have chosen the same potential as that of Williamson and McDowell (1965). Hence we solve (5) after replacing $V_{00}(r)$ by $V_{00}(r)-\frac{\alpha(r)}{r^4}$ where $\alpha(r)$ as given by Bethe (1943) runs as

$$\alpha(r) = -\frac{9}{\beta^4}\left[1-\frac{2}{3}e^{-4\beta r}(1+\beta r)^4-\frac{e^{-2\beta r}}{3}\left(1+2\beta r+6\beta^2 r^2+\frac{20}{3}\beta^3 r^3+\frac{4}{3}\beta^4 r^4\right)\right]$$

where $$\beta = \left(\frac{9}{\alpha}\right)^{1/4} \text{ and } \alpha(r) = \alpha = 1.32 a_0^3$$

To solve (5) for $l = 0$ by the variational method of Hulthen (1944), we have used a trial function of the same form as that of Moiseiwitch (1953) i.e. $f_0(r) = \sin K_0 r + (a + be^{-zr})(1-e^{-zr})\cos K_0 r$ where $Z = 1.6875$. The phase-shift is given by $\eta_0 = \tan^{-1} a$.

The values of the parameters a, b are found from the simultaneous equations

$$L = 0 \quad \text{and} \quad \frac{\partial L}{\partial b} = 0$$

where $$L = L_1 + L_2 + L_3$$

with $$L_1 = \int_0^\infty f_0(r_3)\left[\frac{d^2}{dr_3^2} + K_0^2 - V_{00}(r_3)\right] f_0(r_3) dr_3$$

$$L_2 = \int_0^\infty f_0(r_3)\left[-\frac{\alpha(r_3)}{r_3^4}\right] f_0(r_3) dr_3$$

and $$L_3 = -\int_0^\infty\int_0^\infty\int_0^\infty Q_{00}(r_1, r_2, r_3) f_0(r_1) f_0(r_2) dr_1 dr_2 dr_3$$

The integrals occurring in L_1 are simple and easily evaluated. The integrals occurring in L_2 are of the form

$$I_1 = \int_0^\infty \left[\frac{p}{\beta^4 r^4} + \frac{q}{\beta^3 r^3} + \frac{s}{\beta^2 r^2} + \frac{t}{\beta r} + u\right] e^{-(\nu z + 2ik_0)r} dr$$

with

$$p = 6e^{-4\beta r} + 3e^{-2\beta r} - 9$$

$$q = 24e^{-4\beta r} + 6e^{-2\beta r}$$

$$s = 36e^{-4\beta r} + 18e^{-\beta r}$$

$$t = 24e^{-4\beta r} + 20e^{-2\beta r} \text{ and } u = 6e^{-4\beta r} + 4e^{-2\beta r}$$

$$\nu = 0, 1, 2, 3 \text{ or } 4.$$

On simplification we finally get I_1 as the limiting value of the integral $I_1(\epsilon)$ as $\epsilon \to 0$ where

$$I_1(\epsilon) = \left[\begin{array}{l} \left\{ (\nu z)^3 \left(-\frac{1}{2\beta^4} \right) + (\nu z) \left(\frac{6K_0^2}{\beta^4} - \frac{12}{\beta^2} \right) - \frac{8}{\beta} \right\} \\ \\ + i \left\{ \frac{4K_0^4}{\beta^4} - \frac{24K_0}{\beta^2} - (\nu z)^2 \frac{3K_0}{\beta^4} \right\} \end{array} \right] \int_\epsilon^\infty \frac{e^{-\eta r}}{r} \, dr$$

$$+ \left[\begin{array}{l} \left\{ (\nu z)^4 \left(-\frac{1}{\beta^4} \right) + (\nu z) \left(\frac{12K_0^2}{\beta^2} + \frac{12}{\beta^2} \right) + \frac{8}{\beta} \right\} \\ \\ + i \left\{ \frac{8K_0^3}{\beta^4} + \frac{24K_0}{\beta^2} - (\nu z)^2 \frac{6K_0}{\beta^4} \right\} \end{array} \right] \int_\epsilon^\infty \frac{e^{-\eta r}}{r} \, dr$$

$$+ \left[\begin{array}{l} \left\{ (\nu z)^3 \left(\frac{3}{2\beta^4} \right) - (\nu z) \left(\frac{18K_0^2}{\beta^4} \right) \right\} \\ \\ + i \left\{ (\nu z)^2 \left(\frac{9K_0}{\beta^4} \right) - \frac{12K_0^3}{\beta^4} \right\} \end{array} \right] \int_\epsilon^\infty \frac{e^{-\eta r}}{r} \, dr$$

$$+ 4 \int_\epsilon^\infty e^{-\eta r} \, dr + 6 \int_\epsilon^\infty e^{-\eta r} \, dr$$

$$+ \left[\left\{ (\nu z)^2 \left(\frac{5}{\beta^3} \right) + (\nu z) \left(\frac{9}{\beta^2} \right) + \frac{4}{3\beta} + \frac{20}{\beta^3} K_0^2 \right\} + i \left\{ \frac{18K_0}{\beta^2} - (\nu z) \frac{20K_0}{\beta^3} \right\} \right]$$

with $\rho = \nu z + 2iK_0$, $\xi = \rho + 2\beta$, and $\eta = \rho - 4\beta$.

Again I_2 may be written as $-16\pi^2 N^2 I_2$

where,

$$I_2 = \frac{4-8\lambda}{8\mu^3} D_{1,\lambda} D_{2,\lambda} + \frac{4-8\mu}{8\lambda^3} D_{1,\mu} D_{2,\mu} + \frac{4-8\lambda}{(\lambda+\mu)^3} D_{1,\lambda} D_{2,\mu} + \frac{4-8\mu}{(\lambda+\mu)^3} D_{1\mu} D_{2\lambda}$$

$$+ \frac{4\lambda^2 - 2\mu^2 + 8\mu + 2E}{8\mu^3} D_{2,\lambda} D_{2,\lambda} + \frac{4\mu^2 - 2\lambda^2 + 8\lambda + 2E}{8\lambda^3} D_{2,\mu} D_{2,\mu}$$

$$+ \frac{4\lambda^2 + 4\mu^2 - 4\lambda\mu + 8\lambda + 8\mu + 4E}{(\lambda+\mu)^3} D_{2,\lambda} D_{2,\mu} + \left(\frac{8}{(\lambda+\mu)^3} + \frac{1}{\mu^3} \right) D_{2,\lambda} D_{1,\lambda+2,}$$

$$+\left(\frac{8}{(\lambda+\mu)^3}+\frac{1}{\lambda^2}\right)D_{2,\mu}D_{1,2\lambda+\mu}+\left(\frac{4}{(\lambda+\mu)^2}+\frac{1}{\mu^2}\right)D_{2,\lambda}D_{2,\lambda+2\mu}$$

$$+\left(\frac{4}{(\lambda+\mu)^2}+\frac{1}{\lambda^2}\right)D_{2,\mu}D_{2,2\lambda+\mu}-\frac{1}{2\lambda^3}D_{\mu}{}^{\mu}-\frac{1}{2\mu^3}D_{\lambda}{}^{\lambda}-\frac{4}{(\lambda+\mu)^3}(D_{\lambda}{}^{\mu}+D_{\mu}{}^{\lambda})$$

with $$D_{1,\lambda}=\int_0^{\infty}e^{-\lambda r}f_0(r)dr$$

$$D_{2,\lambda}=\int_0^{\infty}re^{-\lambda r}f_0(r)dr$$

and $$D_{\lambda}{}^{\mu}=\int_0^{\infty}e^{-\mu r}f_0(r)\left\{\int_0^{\infty}(r-r_1)e^{-\lambda r_1}f_0(r_1)dr_1\right\}dr$$

RESULTS AND DISCUSSIONS

We have obtained the scattering length A from our S-wave phase-shifts $\eta_0(.0025)=3.1195$ and $\eta_0(.01)=3.0410$ using the modified effective range formula (O'Malley *et al* 1962)

$$k_0\cot\eta_0(k_0{}^2)=-\frac{1}{A}+\frac{\pi\alpha k_0}{3}+\frac{4\alpha k_0{}^2}{3A}\log(1.23k_0\alpha^{\frac{1}{2}})$$

$$+\left(\frac{1}{2}r_0+\frac{\pi\alpha^3}{3}-\frac{\pi\alpha^{3/2}}{3A^2}-\frac{\pi^2\alpha^2}{9A^3}\right)k_0{}^2+\ldots$$

This formula yields $A=1.1400$ compared with Williamson and McDowell's value of 1.146 and the corresponding value 1.132 of LaBahn and Callaway.

TABLE I

Phase-shift values η_0 for the low-energy range is tabulated below

Electron wave No. K_0	Present Authors	Williamson and McDowell
0.05	3 1195	3 082
0.10	3.0410	3.018
0 50	2.514	2.4935
1.00	2.108	1 963

The zero-energy cross section in our case is $16.33\ a_0{}^2$. The recent experimental value by Pack and Phelps (1961) is $19a_0{}^2$. In most recent experiments by Frost and Phelps (1964), zero-energy cross section is found to be $17.49a_0{}^2$ corresponding

to a scattering length of $1{\cdot}18a_0$. Bandel and Golden (1965) have obtained a scattering length of $1{\cdot}15a_0$ corresponding to the cross section of $16\ 6a_0^2$.

In conclusion, we find that taking adiabatic-dipole polarisation effect into consideration, the discrepancy between experimental zero-energy cross section and the corresponding theoretical one is removed to a large extent The disagreement still left may be mainly due to (i) the adiabatic assumption made in the polarisation potential, (ii) the neglect of higher order terms in the polarisation potential, especially the quadrupole one and (iii) the inaccuracy in the ground-state wave function of the helium atom

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